Final Report

Advanced Conceptual Models for Unsaturated and Two-Phase Flow in Fractured Rock - Project 0008673

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Research Objective

The Department of Energy Environmental Management Program is faced with two major issues involving two-phase flow in fractured rock; specifically, transport of dissolved contaminants in the Vadose Zone, and the fate of Dense Nonaqueous Phase Liquids (DNAPLs) below the water table. Conceptual models currently used to address these problems do not correctly include the influence of the fractures, thus leading to erroneous predictions. Recent work has shown that it is crucial to understand the topology, or 'structure' of the fluid phases (air/water or water/DNAPL) within the subsurface. It has also been shown that even under steady boundary conditions, the influence of fractures can lead to complex and dynamic phase structure that controls system behavior, with or without the presence of a porous rock matrix. Complicated phase structures within the fracture network can facilitate rapid transport, and lead to a sparsely populated and widespread distribution of concentrated contaminants; these qualities are highly difficult to describe with current conceptual models. The focus of our work is to improve predictive modeling through the development of advanced conceptual models for two-phase flow in fractured rock.

Research Accomplishments

1) Conducted a detailed evaluation of the experiments used as the basis for our investigative approach. In those experiments, water was invaded into an air-filled, two-dimensional analog fracture network at a variety of flow rates. Results demonstrated the critical control that fracture intersections place on two-phase flow in fracture networks. At low flows, capillary and gravitational forces combined to create a narrow pulsing flow structure that spanned the system vertically. At higher flows, viscous forces acted to remove the pulsation; however, the flow structure remained narrow. The intersections acted to impose a narrow "slender ladder" structure on the flowing phase that did not expand with depth, but instead remained focused. Results were published in *Water Resources Research* [Glass et al., 2003].

2) Evaluated previous work to consider the influence of fracture intersections on network-scale behavior. Eight experiments were conducted in a 2-D analog fracture-matrix network to evaluate the repeatability of flow under nearly identical conditions and to characterize general patterns in flow behavior. Data revealed that flow generally converged to a single fracture with depth. Periods of pathway switching were observed to be more common than periods with steady, constant flow pathways. We noted the importance of fracture intersections for integrating uniform flow and discharging a "fluid cascade", where water advances rapidly to the next capillary barrier, creating a stop and start advance of water through the network. The results of this simple experiment suggest that the interaction of multiple fracture intersections in a network creates flow behavior not generally recognized in popular conceptual and numerical models. Results were published in the *Vadose Zone Journal* [Wood et al., 2004].

3) Evaluated an extensive set of unpublished experiments investigating gravity destabilized flow in fractures. The experiments were conducted over an approximately ten-year period at Sandia National Laboratories, with the first tests beginning in 1989. Experiments conducted in natural and analog materials showed that unsaturated flow in non-horizontal fractures is fundamentally unstable and forms narrow gravity-driven fingers. At low steady flow, fingers were observed to exhibit pulsation induced by competition between gravitational and capillary forces. This pulsation occurs on a smaller scale than we observed in our experiments that considered flow at fracture intersections. Contrary to studies of infiltration into porous media, gravity-driven flow was not stabilized by the presence of initial moisture within the fractures. A simple scale analysis was also developed to relate the key measures of finger width, finger velocity, and finger length. The scale analysis demonstrated the importance of dynamic capillary pressure in determining finger behavior. Results were published in the *Vadose Zone Journal* [Nicholl and Glass, 2005].

4) Conducted an extensive review of models for fracture networks. These include models developed from observations of networks on outcrops at several scales and stochastic models that are prevalent in the literature from the 1980s to very recent

developments. The results of this investigation were included as part of a review paper that was published in *Reviews in Geophysics* [Molz et al., 2004].

5) Collaborated with a research group led by Dr. Kang-Kun Lee at Seoul National University to consider the effects of groundwater flow on DNAPL migration in fracture networks. A combined experimental-numerical investigation demonstrated that modification of an Invasion Percolation algorithm to include gravity and the first-order effects of viscous forces showed good agreement with physical experiments in a simplistic fracture network. Results were published in *Geophysical Research Letters* [Ji et al., 2003].

6) Sponsored an extended visit to Sandia National Laboratories by Sung-Hoon Ji, a Ph.D. student advised by Dr. Kang-Kun Lee at Seoul National University. Mr. Ji was very active in our laboratory investigation of two-phase flow at individual intersections. The first experiments uncovered fundamental differences between the invasion of water into an air filled intersection and the invasion of a DNAPL into the same intersection under water filled conditions. For a simple intersection between vertical and horizontal fractures, the intersection acted as a capillary barrier to unsaturated flow. Water accumulated above the barrier, then filled the horizontal fractures before continuing downwards in pulses defined by the barrier. Conversely, the TCE did not invade either horizontal fracture, but instead pooled across the intersection to form a capillary bridge that facilitated downwards migration. Results were presented at the 2003 Fall meeting of the American Geophysical Union [Ji et al., 2003] and published in *Geophysical Research Letters* [Ji et al., 2004].

7) Based on the results from item 6 (above), we designed additional experiments to further explore the substantial differences in behavior between wetting (water into air) and nonwetting (TCE into water) flow at intersections between horizontal and vertical fractures. The relative aperture of the horizontal and vertical fractures was varied between trials. In general, capillary barriers to flow formed above all of our intersections for wetting phase flow, while nonwetting phase flows entered the intersection. As a result, wetting phase flows always invaded the horizontal fracture when the capillary barrier breached. Conversely, nonwetting phase flows would not enter a horizontal fracture unless it had a larger aperture than the vertical fracture. These differences have important implications with respect to the spatial and temporal structure of network scale flows. Results have been accepted for publication in *Water Resources Research* [Ji et al., 2006].

8) In collaboration with unsaturated fractured rock research at the Idaho National Laboratory, we evaluated unit processes active at the scale of individual intersections that may explain dynamical behavior observed in experiments at the network scale (see items 1 and 2 above). The competition between capillary, gravitational, viscous, and in some cases inertial forces results in unstable pooling of fluid above intersections. The release of fluid from the pools was seen to be sensitive to both intersection geometry and steady flow rate. Results were presented at the 2004 Fall

meeting of the American Geophysical Union [Wood et al., 2004] and published in *Water Resources Research* [Wood et al., 2005].

9) Slender transport pathways have been found in laboratory and field experiments within unsaturated fractured rock (see items 1 and 2 above). We considered the simulation of such structures with a Modified form of Invasion Percolation (MIP). Results show that slender pathways form in fracture networks for a wide range of expected conditions, can be maintained when subsequent matrix imbibition is imposed, and may arise even in the context of primarily matrix flow due to the action of fractures as barriers to inter-matrix block transport. Results were published in *Geophysical Research Letters* [Glass et al., 2004].

10) A simple model was formulated to explore spatio-temporal structure within regular networks of fracture intersections. Our experiments (see items 6-8) show that individual fracture intersections can impose temporal structure (pulsation) on unsaturated flow by first accumulating and then releasing stored fluid. Spatial structure may result when flow splits, combines, or alternates between outlets at an intersection. The model considers network-scale behavior by treating fracture intersections as tipping buckets. Water enters the network from the top, travels down a fracture, and then stops at the first bucket. When the bucket becomes full, the stored fluid is released into the fractures below. In simulations where all intersections split their outflow between the outlet fractures, the macroscopic flow field diverges with depth and develops into a self-organized dynamical state where the distribution of avalanche sizes follows a power-law over many decades. As the fraction of intersections that direct outflow in a single fracture is increased, spatial structure passes from divergent through braided to a fully convergent, hierarchical flow regime where avalanche size is minimized along one-dimensional slender pathways. Results were published in *Geophysical Research Letters* [Glass and LaViolette, 2004].

11) The tipping bucket model introduced in item 10 (above) carried an assumption that individual intersections would either split or not split their outflow independent of the volume of fluid entering from above. Our experimental evidence suggests that intersection behavior will be dependent on flow rate. At low flows, intersections may release fluid into the single exiting fracture that has the lowest capillary entry pressure. As flow rate is increased, that exit conduit may become overloaded, forcing flow to seek alternate exits and thus lead to flow path splitting. To explore this situation, the tipping bucket model was modified to include "dynamic overloading", where inflow to a bucket that exceeds capacity by more than a specified overload parameter will cause the bucket to split its outflow rather than direct it into a single outlet. With dynamic overloading, the flow behavior transitioned smoothly from diverging to converging with increasing overload parameter. Dynamic overloading also leads to the formation of ephemeral pathways as observed in experiment. Results were published in *Geophysical Research Letters* [LaViolette and Glass, 2004].

12) Added microbial degradation to the tipping bucket model. Our experiments suggest that unsaturated flow moves relatively quickly along fractures and may be temporarily stored at some intersections. The intersections are therefore likely sites for microbial degradation. The tipping bucket model with dynamic overloading was modified to simulate degradation within the buckets. The nature of the flow field was found to have a first-order effect on overall contaminant removal. An order-of-magnitude increase in the degradation rate of the individual, dynamic traps in the flow translated into much smaller increases in the overall reduction of contaminant concentration in the exiting flow. The strongest reductions in contaminant concentration, up to one-third, were found in the systems that supported diverging flow, while the weakest, almost negligible reduction was found in the system that supported converging flow. Results were published in the *Journal of Physical Chemistry B* [LaViolette et al., 2004].

13) Experiments suggest that fracture intersections may combine to impose complicated spatial and temporal dynamics on unsaturated flow at the network scale. Our numerical simulations (see items 10-12 above) imply that networks of intersections may reach a critical state, where discharge of stored fluid from a single intersection triggers a fluid cascade that crosses multiple intersections to rapidly span the system. In collaboration with other research at the Idaho National Laboratory on unsaturated flow in fractured rock we conducted experiments in a mesoscale fracture-matrix network. The analog network was created by stacking 200 cut limestone blocks (15.2 x 5.6 x 4.7 cm each) into 10 vertical columns. The blocks were separated from one another with 0.0762 cm thick spacers to create a network of 9 vertical fractures, 19 horizontal fractures, and 171 fracture intersections. A set of five experiments were conducted. In each experiment, inflow to the top of the fracture network was held constant and outflow from the bottom of the network was measured at all fractures as a function of time. Each trial lasted several days, and the supply rate was varied between trials. We are currently evaluating the data streams that were obtained from these experiments and expect to have a manuscript documenting the outcomes ready for submission to *Water Resources Research* by the end of 2006.

14) Collaborated with investigators at the Idaho National Laboratory (J.M. Hubbell, J.B. Sisson) to evaluate their isobaric well design. Water table gradients at the Idaho National Laboratory are unusually small due to the extremely high saturated hydraulic conductivity of connected fractures within the basalts. As a result, small errors in measurement of water table elevation, such as those associated with fluctuations in barometric pressure can lead to erroneous predictions of hydraulic gradients, flow velocity, flow direction, and contaminant migration. We found that this new isobaric well design significantly reduces the deleterious effects of barometric fluctuations on water level measurements. Results were published in the *Vadose Zone Journal* [Hubbell et al., 2004a].

15) Collaborated with investigators at the Idaho National Laboratory (J.M. Hubbell, J.B. Sisson, D.L. McElroy) to evaluate the potential for estimating liquid flux at depth in a thick vadose zone consisting of fractured basalt. Shallow estimates of flux are

limited by the high degree of spatial and temporal variability present in the near-surface environment. Data from deep tensiometers situated in laterally extensive sedimentary units below and around the Subsurface Disposal Area at the Idaho National Laboratory suggested a much more stable monitoring environment. This approach was found to be limited by a high degree of uncertainty in the estimation of unsaturated hydraulic properties from deep core samples. Results were published in the *Vadose Zone Journal* [Hubbell et al., 2004b].

16) Collaborated with investigators at the Idaho National Laboratory (J.M. Hubbell, J.B. Sisson) and the University of Idaho (J. Osiensky) to evaluate a new Idaho National Laboratory design for a suction bailer. Our research has shown that flow through unsaturated fractured rock can follow slender converging pathways (see items 1 and 2 above), making it difficult to sample. Sedimentary units located within the unsaturated fractured basalts at the Idaho National Laboratory may interrupt such pathways and provide an opportunity to sample flow that spreads laterally. This new bailer was shown to be a robust design that is capable of sampling water layers that are as thin as 1 cm. Results were published in the *Vadose Zone Journal* [Hubbell et al., 2006].

17) Collaborated with J.M. Hubbell, at the Idaho National Laboratory to develop a new technique for measuring liquid flux in the deep vadose zone. The research described in item 15 (above) concluded that sedimentary layers within the thick unsaturated basalts below the Subsurface Disposal Area at the Idaho National Laboratory were amenable to measurement of vertical flux. However, conventional means of estimating the unsaturated hydraulic conductivity were also identified as a substantial limitation. To meet that need, a laboratory method for measuring unsaturated conductivity at the ambient moisture content was developed. Measurement apparatus was constructed and tested on two samples of local material. Results show considerable promise, and are currently being developed into a manuscript for submission to the *Vadose Zone Journal* by the end of 2006.

18) Collaborated with R.M. Holt at the University of Mississippi to develop a special section of the *Vadose Zone Journal* dedicated to the topic of uncertainty in vadose zone flow and transport prediction. The special section includes eight refereed articles and an introduction to the topic [Holt and Nicholl, 2004].

Refereed Publications Resulting From This Project

Glass, R.J., M.J. Nicholl, H. Rajaram, and T.R. Wood, Unsaturated flow through fracture networks: Evolution of liquid phase structure, dynamics, and the critical importance of fracture intersections, *Water Resources Research*, 39(12), 1352, doi:10.1029/2003WR002015, 2003.

Glass, R.J., M.J. Nicholl, H. Rajaram, and B. Andre, Development of slender transport pathways in unsaturated fractured rock: Simulation with modified invasion percolation, *Geophysical Research Letters*, 31, L06502, 2004.

Glass, R.J. and R.A. LaViolette, Self organized spatial-temporal structure within the fractured vadose zone: Influence of fracture intersections, *Geophysical Research Letters*, 31, L15501, doi:10.1029/2004GL019511, 2004.

Holt, R.M. and M.J. Nicholl, Uncertainty in vadose zone flow and transport prediction, *Vadose Zone Journal*, 3, 580-584, 2004.

Hubbell, J.M., J.B. Sisson, M.J. Nicholl, and R.G. Taylor, Well design to reduce barometric pressure effects on water level data in unconfined aquifers, *Vadose Zone Journal*, 3, 183-189, 2004a.

Hubbell, J.M., M.J. Nicholl, J.B. Sisson, and D.L. McElroy, Estimating flux in a deep vadose zone using the Darcian approach, *Vadose Zone Journal*, 3, 560-569, 2004b.

Hubbell, J.M., J.L. Osiensky, M.J. Nicholl, and J.B. Sisson, A suction bailer for sampling very thin saturated zones, *Ground Water Monitoring and Remediation*, 26(2), 52-57, 2006.

Ji, S.H., I.W. Yeo, K.K. Lee, and R.J. Glass, Influence of ambient groundwater flow on DNAPL migration in a fracture network: Experiments and simulations, *Geophysical Research Letters*, 30(10), 11-1 to 11-4, doi:10.1029/2003GL017064, 2003.

Ji, S-H., M.J. Nicholl, R.J. Glass, and K-K. Lee, Influence of a simple fracture intersection on density-driven immiscible flow: Wetting vs. nonwetting flows, *Geophysical Research Letters*, 31, L14501, doi:10.1029/2004GL020045, 2004.

Ji, S-H., R.J. Glass, and K-K. Lee, Influence of simple fracture intersections with differing aperture on density-driven immiscible flow: Wetting vs. nonwetting flows, accepted for publication in *Water Resources Research*, 2006.

LaViolette, R.A. and R.J. Glass, Self organized spatio-temporal structure within the fractured vadose zone: The influence of dynamic overloading at fracture intersections, *Geophysical Research Letters*, V. 31, L18501, doi:10.1029/2004GL020659, 2004.

LaViolette, R.A., R.J. Glass, D. Peak, and D.L. Stoner, Self-organized network of chemical reactions: A model of contaminated converging and diverging flows in fractured media, *J. Phys. Chem. B*, 108 (51), 19657 -19662, 2004. 10.1021/jp0476500 S1089-5647(04)07650-3, 2004.

Molz, F.J., H. Rajaram, and S.L. Lu, Stochastic fractal-based models of heterogeneity in subsurface hydrology: Origins, applications, limitations, and future research questions, *Reviews of Geophysics*, 42(1), RG1002, 2004.

Nicholl, M.J. and R.J. Glass, Infiltration into an analog fracture: Experimental observations of gravity-driven fingering, *Vadose Zone Journal*, 4, 1123-1151, 2005.

Wood, T.R., R.J. Glass, R.A. LaViolette, D.L. Stoner, T.R. McJunkin, R.K. Podgorney, K.S. Noah, R.C. Starr and K.E. Baker, Unsaturated flow through a small fracture-matrix network: Part 1, experimental observations, *Vadose Zone Journal*, 3, 90-100, 2004.

Wood, T.R., M.J. Nicholl, and R.J. Glass, Influence of fracture intersections under unsaturated, low flow conditions, *Water Resources Research*, 41, W04017, 2005.

Published Abstracts Resulting From This Project

Ji. S-H., M.J. Nicholl, R.J. Glass, and K-K. Lee, The role of fracture intersections on DNAPL migration below the water table, Fall 2003 Meeting of the American Geophysical. Union, San Francisco, CA, (H42F), EOS, 84(46), 2003.

Wood, T.R., M.J. Nicholl, and R.J. Glass, Influence of fracture intersections under unsaturated, low flow conditions, Fall 2004 Meeting of the Am. Geophys. Union, San Francisco, CA, (H43F), EOS, 85(47), 2004.